# SUPPORTING INFORMATION

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# Competition among $Li^+$, $Na^+$, $K^+$ and $Rb^+$ Monovalent Ions for DNA in Molecular Dynamics Simulations using the Additive CHARMM36 and Drude Polarizable Force Fields

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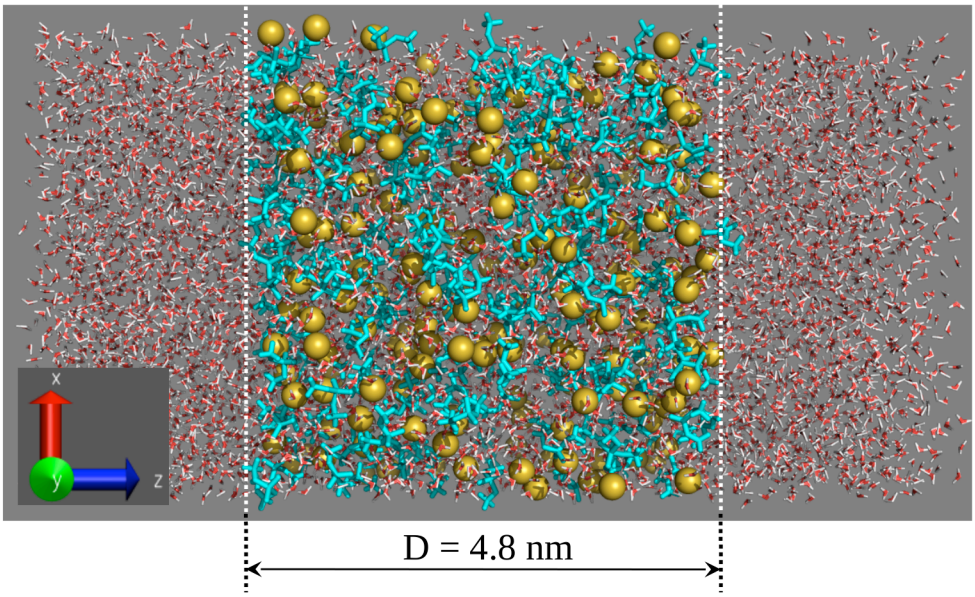


**Figure S1.** Snapshot from MD simulation of the ~1M aqueous solution of the $DMP^-$ and $Na^+$ ions. Sodium ions are yellow, DMP ions are cyan, water is red/white.

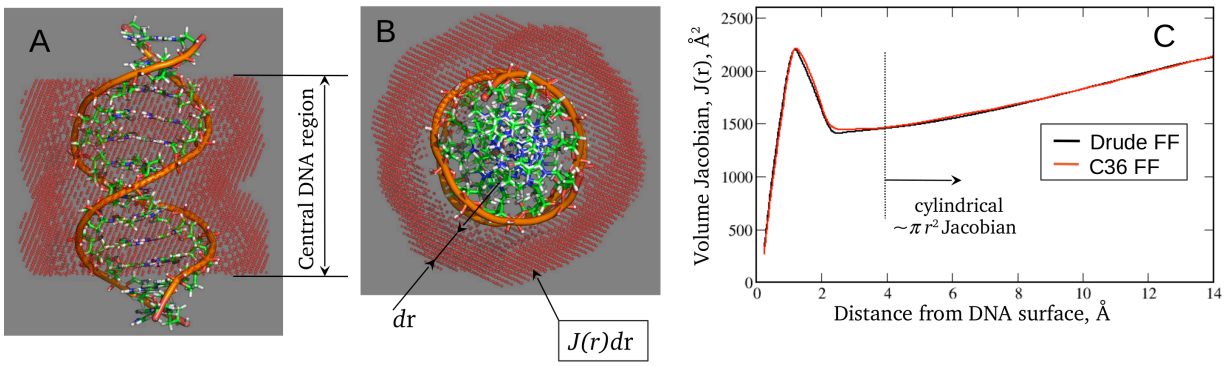


**Figure S2.** Side (A) and top (B) views of the DNA and equidistant shell (in red) from its surface. The shell's thickness is *dr* and its volume is *J(r)dr*. *J(r)* is the volume Jacobian whose numerical value as a function of the distance from DNA surface is shown in C. It is seen that only after ~4 Å from the DNA does the function start to increase monotonically and, thus, in this region can be approximated by the cylindrical Jacobian often used for calculation of the ionic distributions around DNA. To avoid end effects, ionic distributions were analyzed in the central region of the DNA, as shown in A.

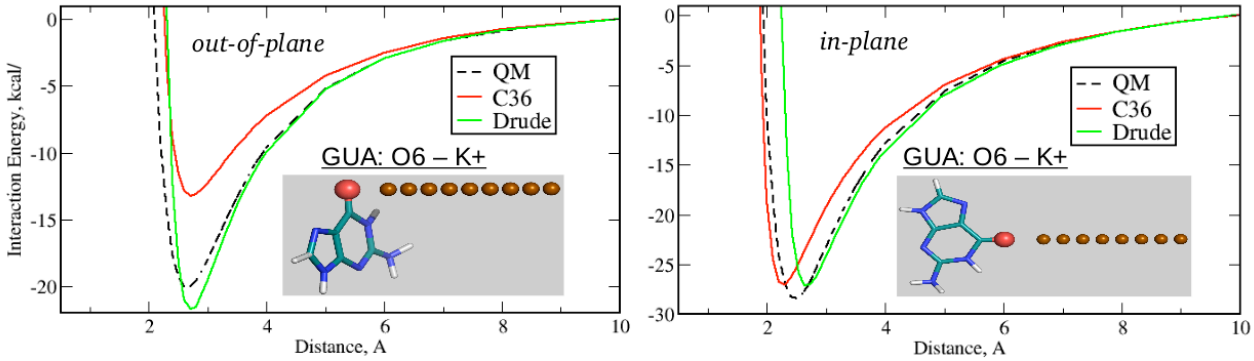


**Figure S3.** QM and empirical Drude and C36 potential energy surfaces as functions of the distance between $K^+$ ion and O6 atom of the guanine base in the in-plain and out-of-plane orientations.

**Table S1.** Final LJ parameters in the NBFIX format for the Drude and C36 models[a]

| | $Li^+$ | | $Na^+$ | | $K^+$ | | $Rb^+$ | |
|---|---|---|---|---|---|---|---|---|
| | **Drude FF** | | | | | | | |
| | $\varepsilon$ | $R_{ij}$ | $\varepsilon$ | $R_{ij}$ | $\varepsilon$ | $R_{ij}$ | $\varepsilon$ | $R_{ij}$ |
| $Cl^-$ | -0.0464 | 3.800 | -0.0476 | 4.090 | -0.1010 | 4.210 | -0.1402 | 4.270 |
| OD2C2C | -0.0458 | 3.135 | -0.0470 | 3.496 | | | | |
| OD30BN | -0.0245 | 3.020 | -0.0251 | 3.382 | | | | |
| ND2B1 | -0.0693 | 3.600 | -0.0710 | 3.780 | -0.1506 | 3.800 | -0.2090 | 3.800 |
| ND2R6B | -0.0548 | 3.600 | -0.0560 | 3.790 | -0.1191 | 3.800 | -0.1652 | 3.820 |
| ND2R6C | -0.0612 | 3.600 | -0.0627 | 3.620 | -0.1332 | 3.700 | -0.1847 | 3.700 |
| | **CHARMM36 FF** | | | | | | | |
| $Cl^-$ | -0.0187 | 3.6875 | -0.0839 | 3.731 | -0.1142 | 4.081 | | |
| ON3 | -0.0167 | 3.1775 | | | | | | |

[a]Atom names correspond to the CHARMM Drude and C36 topology files.

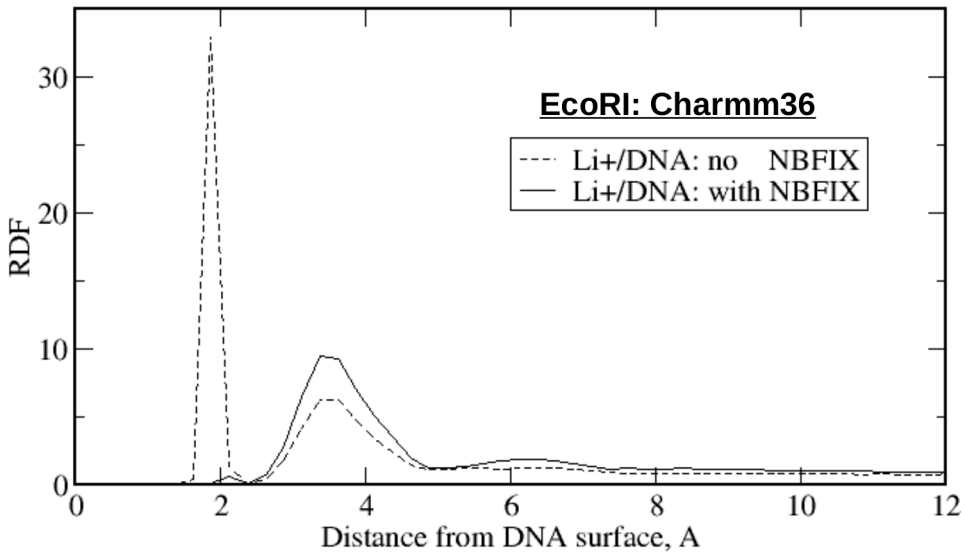


**Figure S4.** Effect of the NBFIX modification on the overall distribution of $Li^+$ around DNA.

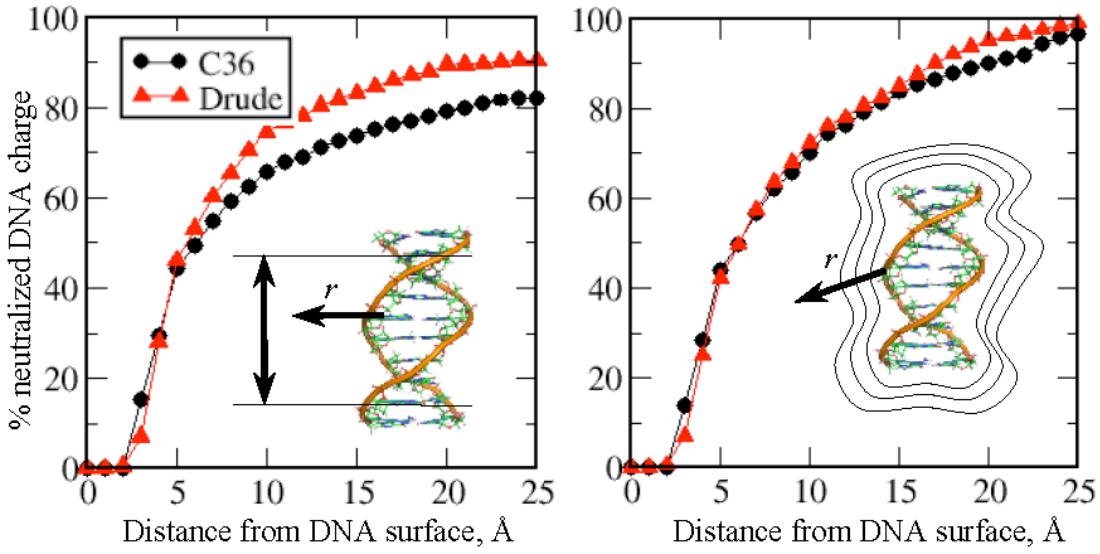


**Figure S5.** Percent fraction of the DNA charge neutralized by all ions as a function of distance from DNA computed by averaging over the central part of the molecule (left) and over the entire region around the DNA (right).